Numerical Study of the Spin-Flop Transition in Anisotropic Spin-1/2 Antiferromagnets

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(Dated: February 1, 2008)

Magnetization processes of the spin-1/2 antiferromagnetic XXZ model in two and three spatial dimensions are studied using quantum Monte Carlo method based on stochastic series expansions. Recently developed operator-loop algorithm enables us to show a clear evidence of the first-order phase transition in the presence of an external magnetic field. Phase diagrams of closely related systems, hard core bosons with nearest-neighbor repulsions, are also discussed focusing on possibilities of phase-separated and supersolid phases.

PACS numbers: 75.10.-b, 75.10.Jm, 74.20.Mn

There have been a lot of interests on magnetic properties of anisotropic quantum antiferromagnets since Néel first predicted the first-order phase transition in the presence of an external magnetic field [1]. One of the simplest models for anisotropic antiferromagnets in an external magnetic field is described by the following spin-1/2 XXZ model Hamiltonian:

$$H = J\sum_{\langle \mathbf{i},\mathbf{j}\rangle}\left(S^x_{\mathbf{i}}S^x_{\mathbf{j}} + S^y_{\mathbf{i}}S^y_{\mathbf{j}} + \Delta S^z_{\mathbf{i}}S^z_{\mathbf{j}}\right) - h\sum_{\mathbf{i}} S^z_{\mathbf{i}}, \quad (1)$$

where $S^\alpha_{\mathbf{i}}$ is the $\alpha(= x, y, z)$ component of the spin-1/2 operator at site $\mathbf{i}$, h is an external magnetic field applied in the z-direction, and $\langle \mathbf{i},\mathbf{j}\rangle$ runs over all the nearest-neighbor pairs of spins at sites $\mathbf{i}$ and $\mathbf{j}$. $J(> 0)$ is antiferromagnetic coupling and $\Delta(\geq 0)$ is anisotropic constant. Mean-field calculations of the spin-1/2 XXZ model [2], supporting Néel's prediction, found the first-order phase transition from the Néel ordered state to the spin-flopping state with increasing the magnetic field h. On the contrary to these studies, it is known from Bethe ansatz solution that the one-dimensional (1D) spin-1/2 XXZ model shows a second-order transition in the presence of the external magnetic field [3]. The discrepancy is assigned to the inadequacy of treating quantum fluctuations by the mean-field theories. It is thus important to use an unbiased numerical method for understanding the correct nature of the magnetization process even for the simplest systems such as one given by Eq. (1) in higher spatial dimensions since there exist no analitically exact solutions. This is preciely one of our purposes for this paper [4].

Another importance of studing the spin-1/2 XXZ model defined by Eq. (1) comes from the fact that the model is mapped onto a system of hard core bosons with nearest-neighbor repulsions described by the Hamiltonian

$$H_{\mathrm{B}} = -t\sum_{\langle \mathbf{i},\mathbf{j}\rangle}\left(c^\dagger_{\mathbf{i}}c_{\mathbf{j}} + c^\dagger_{\mathbf{j}}c_{\mathbf{i}}\right) + V\sum_{\langle \mathbf{i},\mathbf{j}\rangle} n_{\mathbf{i}}n_{\mathbf{j}} - \mu\sum_{\mathbf{i}} n_{\mathbf{i}}, \quad (2)$$

with $t = J/2$, $V = J\Delta$, and $\mu = h + zJ\Delta/2$ (z: coordination number)[5]. Here $c^\dagger_{\mathbf{i}}$ is a creation operator of hard core boson at site $\mathbf{i}$ and $n_{\mathbf{i}} = c^\dagger_{\mathbf{i}}c_{\mathbf{i}}$. The total magnetization $M_z = \sum_{\mathbf{i}} S^z_{\mathbf{i}}$ thus relates to $\sum_{\mathbf{i}}(n_{\mathbf{i}} - 1/2)$ in the boson model. The boson Hamiltonian H_{B} is proposed as a model Hamiltonian to study properties of liquid ^{4}He [6], granular superconducting arrays [7], and flux lines in superconductors [8]. The ground state phase diagram has been studied using mean-field theories [2, 9] and numerical methods [10], and shows a Mott insulating phase, a superfluid phase, and a phase with having both the orders simultaneously (*supersolid* phase). The correspondence of these states to those in the spin model is as follows: Mott insulating and Néel states, superfluid and spin-flopping states, and supersolid and "intermediate" spin states [2], respectively.

The main purpose of this paper is to show a clear evidence for the first-order phase transition of the 2D and 3D spin-1/2 XXZ models in the presence of a magnetic field by using recently developed numerical method and present the ground state phase diagrams. The presence of a phase-separated phase and the absence of the supersolid phase in the closely related system of hard core bosons with nearest-neighbor repulsions are also discussed.

The magnetization process of the 2D and 3D spin-1/2 XXZ models defined by Eq. (1) is studied numerically on square (number of spins $N_s = L \times L$) and cubic ($N_s = L \times L \times L$) lattices using quantum Monte Carlo (QMC) technique based on stochastic series expansions (SSE) [11]. Very recently an important technical improvement have been achieved by Sandvik [12]. He found a new algorithm of cluster-type updates (operator-loop updates) within the SSE QMC scheme which reduces autocorrelation time drastically compared to simulations using only local updates. While this method is very similar to the loop algorithm in the world-line QMC method proposed by Evertz *et al.* [13], one major advantage of the SSE method with operator-loop updates is that there is no difficulty in simulating systems with anisotropic couplings in external magnetic fields owing to not having to have "freezing" configurations and "global" weights which make the loop algorithm in the world-line QMC method highly inefficient [12]. This reduced autocorrelation time enables us to go down to very low temperatures

in very high magnetic fields and therefore the method is suitable for our purpose. Another advantage of this study using the SSE scheme over other earlier numerical studies [4, 10, 14] is that the simulations are performed directly in the ground canonical ensemble, *i.e.*, magnetization per site $m_z = M_z/N_s$ is calculated for a given magnetic field h. In this paper temperatures T are set to be $J/k_{\rm B}T = 2L$ which is low enough to study the ground state properties on finite lattices [15], and periodic boundary condition is used. The exchange coupling J will be taken as the energy unit. Since there exists long-range Néel-ordered state only for $\Delta \geq 1.0$, from which the first-order spin-flop transition can take place by applying a finite external field, our main focus in this paper will be put on this anisotropic regime.

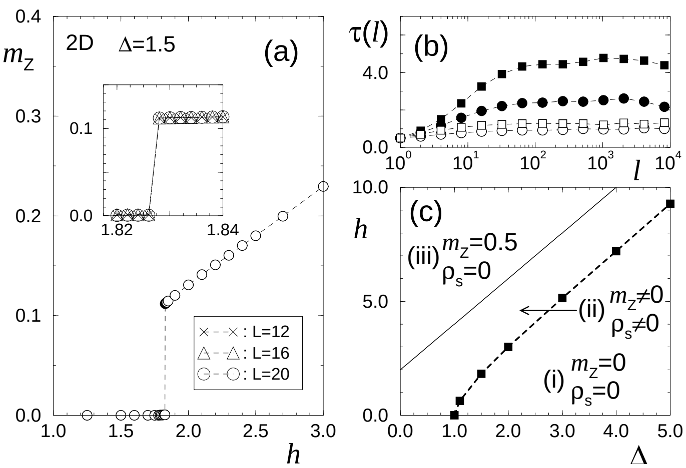

FIG. 1: (a) Magnetization curve of the 2D spin-1/2 XXZ model with $\Delta = 1.5$. Inset: enlarged scale is used. Error bars are smaller than symbols. (b) Correlation time $\tau(l)$ (for definition see in the text) of m_z (circles) and $S(\pi,\pi)$ (squares) as a function of bin length l. The parameters are $N_s = 12^2$, $T = 1/24$, $\Delta = 1.5$, and $h = 2.0$. Solid (open) marks are data for operator-loop updates with closed loops constructed as many as 25 (100) times per MC step. (c) The ground state phase diagram of the 2D spin-1/2 XXZ model with anisotropic constant Δ in the presence of the magnetic field h. There exist three phases: (i) Néel ordered phase, (ii) spin-flopping phase, and (iii) fully saturated ferromagnetic phase. Solid line is $2(1+\Delta)$ (see in the text). Dashed line is a guide to the eye.

Let us first study the magnetization process in 2D. A typical example of the magnetization curves is shown in Fig. 1 (a). One can see that at certain critical magnetic field h_c the magnetization m_z changes discontinuously from 0 to a finite value m_z^c. For this example in the figure with $\Delta = 1.5$ the magnetization jumps at $h_c \sim 1.83$ to $m_z^c \sim 0.11$ [16]. Working on various system sizes (see in the inset of Fig. 1(a)), we confirm that finite size effects are small and conclude that the jump in magnetization is not due to extrinsic factors of working on finite-size lattices. The result already gives a clear evidence for the first-order phase transition.

In order to illustrate that autocorrelation times of our QMC measurements are short enough, the integrated autocorrelation time $\tau_{\rm int}$ is estimated as follows: we first divide a sequence of Monte Carlo data points into bins of length l, and for each bin length l, the average of the data in the bth bin and the variance $\sigma^2(l)$ of the bin averages are calculated. The integrated autocorrelation time $\tau_{\rm int}$ is then estimated by the asymptotic value of $\tau(l) = l\sigma^2(l)/2\sigma^2(l=1)$ at large l above which $\tau(l)$ does not depend on l [17]. The results of $\tau_{\rm int}$ for m_z and spin structure factor $S(\mathbf{q})$ at $\mathbf{q} = (\pi,\pi)$ are shown in Fig. 1 (b) for $\Delta = 1.5$ and $h = 2.0$. From this figure $\tau_{\rm int}$'s are estimated to be no longer than 4–5 MC steps. Since we use bin length $l = 1000$ or more to estimate the statistical errors, we can be sure that our error bar is accurate. It should be noted here that $\tau_{\rm int}$ can be controlled by changing how many times closed loops are constructed in the operator-loop updates. In this paper we have to construct closed loops as many as about 1000 times per MC step for larger values of Δ.

Repeating the same procedure for different values of Δ, the ground state phase diagram of the 2D spin-1/2 XXZ model is completed. The result is given in Fig. 1 (c). There exist three different phases denoted by (i) $m_z = 0$, (ii) $m_z \neq 0$, and (iii) $m_z = 0.5$ in the Figure. The third phase (iii) corresponds to a fully saturated ferromagnetic phase and is separated from the second phase (ii) by the critical magnetic field $h_c^{\rm max}$. This transition is trivial and is not our interest here. The critical magnetic field $h_c^{\rm max}$ is indeed easily calculated by going to the boson model described by Eq. (2): the critical chemical potential to have just one particle in the d-dimensional boson system is $-2dt$ and therefore $h_c^{\rm max}/J$ is found to be $d(1+\Delta)$.

To show further evidence for the first-order transition between phase (i) and phase (ii) we calculate the spin structure factor $S(\mathbf{q}) = 1/N_s \sum_{\mathbf{i},\mathbf{j}} e^{i\mathbf{q}\cdot(\mathbf{i}-\mathbf{j})}\mathbf{S_i}\cdot\mathbf{S_j}$ at $\mathbf{q} = (\pi,\pi)$ and the spin stiffness (helicity modulus) ρ_s as a function of h for a fixed Δ. The spin stiffness ρ_s is calculated by, for example, $\rho_s = T\langle w_x^2 + w_y^2(+w_z^2)\rangle/dL^{d-2}$ in 2D (3D) where w_α is the winding number per linear spatial lattice size L in the α-direction [18]. ρ_s corresponds to the superfluid density in the boson model and is used to detect the superfluid phase in the system [9, 10, 18]. The results are shown in Fig. 2(a) for $\Delta = 1.5$ as a function of h. When h is small $S(\mathbf{q})$ has a peak at $\mathbf{q} = (\pi,\pi)$ ($\mathbf{q}$ dependence is not shown) and $\rho_s = 0$. With increasing h these quantities change discontinuously at h_c where the magnetization m_z jumps, and $S(\pi,\pi)$ becomes zero while ρ_s has a finite value [19]. Apparently these two phases are (i) Néel ordered phase (for $h < h_c$) and (ii) spin-flopping phase (for $h > h_c$), and are separated through the first-order transition [20].

Earlier studies found the supersolid phase in the boson model characterized by having finite values of $S(\pi,\pi)$ and ρ_s simultaneously in a region between phase (i) and phase (ii) of the phase diagram [9, 10]. One can indeed barely see small but finite values of $S(\pi,\pi)$ for $h > h_c$ where ρ_s is finite (see Fig.2 (a)). In order to elucidate systematically the possibility of the existence of the supersolid phase

in 2D, we carry out the finite size scaling analyses of $S(\pi,\pi)$ and ρ_s for fixed magnetizations. The results are presented in Fig. 2(b). One can see that $S(\pi,\pi)/N_s$ (ρ_s) stays finite in the limit of $N_s \to \infty$ for $h < h_c$ ($h > h_c$) while $S(\pi,\pi)/N_s$ approaches to zero at $N_s \to \infty$ for $h > h_c$. Doing the similar analyses for different values of Δ and m_z it is found that whenever $h > h_c$ $S(\pi,\pi)/N_s$ goes to zero in the thermodynamic limit. We therefore conclude that the supersolid phase does not exist in the 2D spin-1/2 XXZ model. The results are consistent with very recent studies by Batrouni and Scalettar [14].

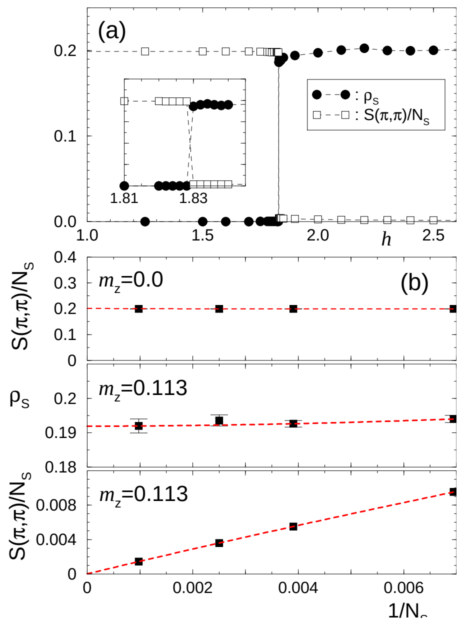

FIG. 2: (a) $S(\pi,\pi)$ and ρ_s for the 2D spin-1/2 XXZ model with $\Delta = 1.5$ and $N_s = 20^2$ as a function of the magnetic field h. Inset: enlarged scale is used. (b) Finite size scaling of $S(\pi,\pi)/N_s$ and ρ_s for different magnetizations with $\Delta = 1.5$. The top figure shows $S(\pi,\pi)/N_s$ for $m_z = 0$ and the middle (bottom) figure shows ρ_s ($S(\pi,\pi)/N_s$) for $m_z = 0.113$. Dashed lines are liner fitting curves of QMC data, extrapolating to $1/N_s \to 0$.

We now carry out the similar calculations for the 3D spin-1/2 XXZ model to study the nature of the phase transition induced by the external magnet field. Our strong evidence for the first-order transition is provided in Fig. 3(a). In the Figure magnetization m_z, spin structure factor $S(\pi,\pi,\pi)$, and spin stiffness ρ_s for $\Delta = 1.5$ are plotted as a function of the external magnetic field h. It is clearly seen that as in the case of the 2D model those quantities change discontinuously at the critical magnetic field h_c. Working with different values of Δ, the ground state phase diagram is constructed and the result is shown in Fig. 3(b). As in 2D the phase diagram consists of three different phases: (i) Néel ordered phase, (ii) spin-flopping phase, and (iii) fully saturated ferromagnetic phase [21]. The critical magnetic field h_c in 3D is observed to be larger compared to that in 2D for a given Δ. This is simply because the increased coordination number in 3D makes the needed magnetic field larger to destroy the Néel state. The similar finite size scaling analyses which was done for the 2D model do not find the supersolid phase in the 3D model.

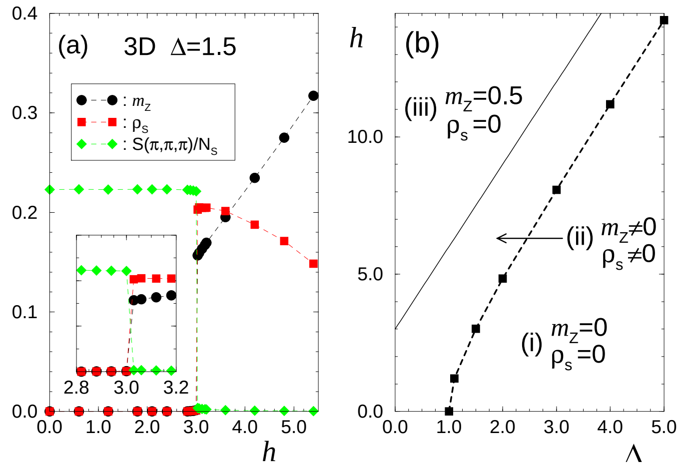

FIG. 3: (a) m_z, $S(\pi,\pi,\pi)$, and ρ_s for the 3D spin-1/2 XXZ model with $\Delta = 1.5$ and $N_s = 8^3$ as a function of the magnetic field h. Inset: enlarged scale is used. (b) The ground state phase diagram of the 3D spin-1/2 XXZ model with anisotropic constant Δ in the presence of the magnetic field h. The diagram consists of (i) Néel ordered phase, (ii) spin-flopping phase, and (iii) fully saturated ferromagnetic phase. Solid line is $3(1+\Delta)$ (see in the text). Dashed line is a guide to the eye.

Finally we summarize our results in Fig. 4 by showing the ground state phase diagrams of the 2D and 3D spin-1/2 XXZ models on the parameter space of anisotropic constant Δ and magnetization m_z. The phase diagrams show (i) the Néel ordered state at $\Delta \geq 1.0$ and $m_z = 0.0$, (ii) the spin-flopping state with $\rho_s \neq 0$, (iii) the fully saturated ferromagnetic state at $m_z = 0.5$, and (iv) a phase-separated state (denoted by PS in the Figures). The phase-separated region exists because as was seen in Figs. 1(a) and 3(a) there is a region in magnetization m_z to which we can not reach in a thermodynamically stable way no matter how fine the magnetic field h is tuned. In other words, if one could have a states with m_z which is in this magnetization region, the state would be phase-separated between the Néel state with $m_z = 0$ and the spin-flopping state with $m_z = m_z^c$. Some earlier studies predicted two phase coexisting regions working with the canonical ensemble (*i.e.*, fixed m_z) and their results were interpreted as the supersolid phase [9, 10]. However our calculations conclude that these phases are thermodynamically unstable and are phase-separated. Our conclusions are consistent with recent studies by Batrouni and Scalettar for the 2D boson model [14].

In conclusion, we have studied numerically the magnetization process of the spin-1/2 anisotropic XXZ model in two and three spatial dimensions using QMC method based on SSE and shown clear evidences of the first-order phase transition in the presence of an external magnetic

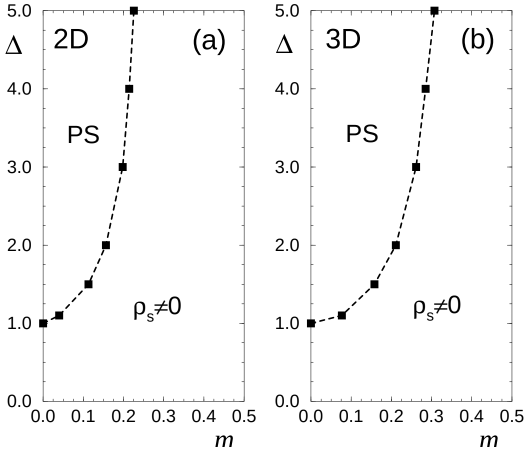

FIG. 4: The ground state phase diagrams of the (a) 2D and (b) 3D spin-1/2 XXZ models on the parameter space of anisotropic constant Δ and magnetization m_z. PS stands for phase separation. The Néel (fully saturated ferromagnetic) sate exists in the region of $\Delta \geq 1.0$ and $m_z = 0.0$ ($m_z = 0.5$). The spin-flopping phase is in the region denoted by $\rho_s \neq 0$. Dashed line is a guide to the eye. For the boson model defined by Eq. (2) m_z and Δ correspond to $0.5 - n$ and $V/2t$, respectively.

field. Based on the calculated ground state phase diagrams, the existence of a phase-separated region and the absence of supersolid phases are pointed out in the related systems of hard core bosons with nearest-neighbor repulsions.

It would be of great interest to study effects of random anisotropic constant Δ on the phase diagrams [22] since one can elucidate *quantum* effects on recently proposed impurity-induced quantum-critical-point-like behavior near $first$-order phase transitions in the Ising models [23]. Another interesting issue to address is to see effects of long-ranged Coulomb repulsions between bosons on the phase-separated region in the phase diagram. There is a general belief that introducing the Coulomb interactions replaces the phase-separated state by thermodynamically stable states such as a droplet-like state and perhaps a stripe state [24]. The model studied here provide an ideal system to examine the possibilities of those exotic states using unbiased numerical methods.

The author thanks E. Dagotto and A. Dorneich for valuable discussions.

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[21] Note in phase (ii) $\langle w_x^2 \rangle = \langle w_y^2 \rangle = \langle w_z^2 \rangle$.
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